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Title: Grain boundary structure of two-dimensional tellurium revealed by 4D STEM

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Intended for: Experiment Brief for Gatan Inc. The company will use our write-up in their promotional materials to demonstrate the capabilities their instruments can enable.
Web

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Experiment Brief

K3 IS Camera and STEMx System

Title

Grain boundary structure of two-dimensional tellurium revealed by 4D STEM

Gatan Instrument Used

The K3™ IS camera delivers simultaneous low-dose imaging via real-time electron counting, fast continuous data capture, and a large field of view (FOV). In a 4D STEM experiment, the STEMx™ system precisely synchronizes the speed of the scanning probe to the camera frame rate to enable high-speed data acquisition and eliminates the potential for data loss.

Background

The recent realization of 2D tellurium (tellurene) has allowed scientists to demonstrate an air-stable monoelemental van der Waals material with remarkable potential for applications in electronics and optoelectronics. The chiral-chain structure of ultrathin Te allows controllable electronic and optical properties due to the non-monotonic carrier mobility and an increase in electronic band-gap as the thickness is reduced. Scalable and accurate production of 2D Te-based functional devices will require detailed knowledge of structural defects and strain field distributions that can be linked to transport properties.

Materials and Methods

A Gatan K3™ IS camera and STEMx™ system was used to capture crystallographic orientations near a grain boundary in 2D tellurene. A set of over ~15,000 diffraction patterns from a 116×133 pixel region was recorded on a FEI Titan ETEM operating at 300 kV with a dwell time of 20 ms per pixel. The collection of machine and software binned 512×512 pixel CBED patterns form a 4D STEM dataset ~8 GB in size within a few minutes, a unique feature enabled by the fast acquisition possible with the K3™ IS. Data processing and image analysis were performed using DigitalMicrograph® software and a suite of custom algorithms for peak finding and real space image reconstruction.

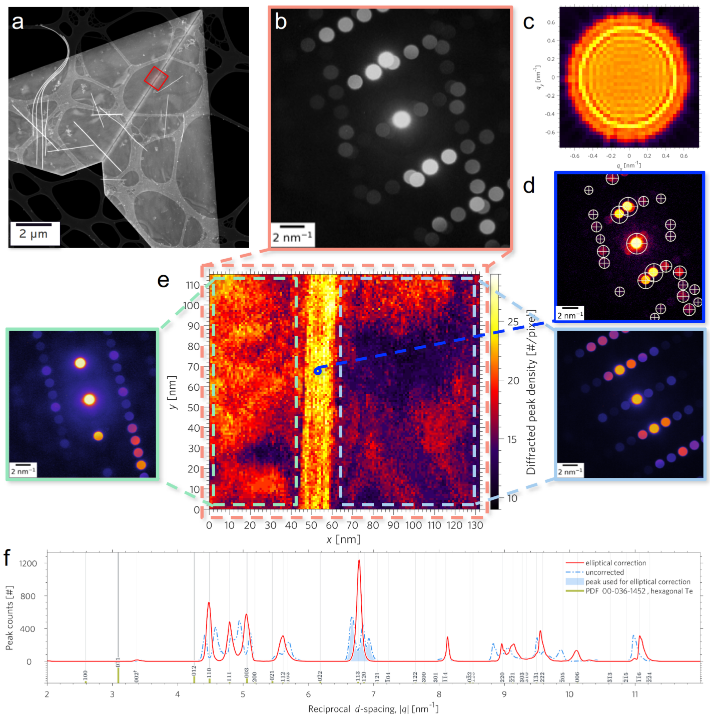

Figure 1. Crystallographic grain boundary classification of 2D tellurene. a) Low magnification STEM image indicating the 116×133-pixel region characterized with STEMx (red rectangle). b) Sum of all 15,428 CBED patterns across the region marked in (a). c) Center beam profile used to locate diffracted peaks. d) Peak identification algorithm results from CBED pattern inside the grain boundary. e) Reconstructed real space image using the diffracted peak density and crystallographic classification clearly shows the ~15nm-thick grain boundary region and two distinct orientations at each side of the boundary. f) Peak histogram of red region in (a) before and after elliptical correction.

Summary

Unlike conventional DF imaging, 4D STEM gives access to the complete information contained within the CBED pattern, allowing for comprehensive post-experiment data analysis by the user. The large size of high quality data sets enabled by the K3™ IS and STEMx™ allowed us to obtain and index the 278,904 uniquely identified diffraction peaks with an uncertainty in the range of $U_q/q = (0.5–1.5)\times10^{-4}$. This in turn allowed us to determine the phase is uniformly hexagonal Te with local unit cell parameters of $a = 4.464(20)$ Å and $c = 5.936(20)$ Å.

Credit(s)

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